Electron Spectroscopy Group at Physics Department, BNL

/ Peter Johnson, Alexei Fedorov, Tonica Valla/

Angle resolved photoemission:

- ✓ High temperature superconductors /$Bi_2Sr_2CaCu_2O_8$, Sr_2RuO_4 /
- ✓ Low-dimensional conductors /CDW, non-Fermi liquid behavior/
- ✓ Two-dimensional conductors /surface states, 2H-$TaSe_2$ /
- ✓ Amorphous films /search for the Coulomb gap/

Spin-polarized photoemission:

- ✓ Micro-Mott detector connected to the Scienta analyzer /surface states in Gd(0001)/

Photoemission Studies of Layered Dichalgonedie
2H-$TaSe_2$
in the Normal and Charge Density Wave States

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Charge Density Waves

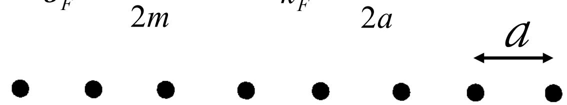
R.E. Peirls, Quantum Theory of Solids (Clarendon, Oxford, 1955); **H. Fröhlich**, Proc. R. Soc. Lond. A 223, 296 (1954); **A.W. Overhauser**, Phys. Rev. 167, 691 (1968); **S.-K. Chan** and **V. Heine**, J. Phys. F 3, 795 (1973)

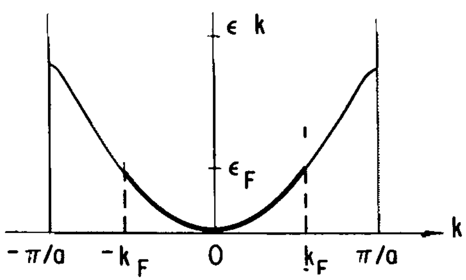
☆ G. Grüner, Density Waves in Solids (Addison-Wesley, Reading, 1994) ☆

1. Lets take one-dimensional electron gas...

$$\varepsilon(k) = \hbar^2 k^2 / 2m$$

$$\varepsilon_F = \frac{\hbar^2 k_F^{\,2}}{2m} \qquad k_F = \frac{N_0 \pi}{2a}$$





2. Consider response of an electron gas to a time independent potential:

$$\phi(\vec{r}) = \int_q \phi(\vec{q}) e^{i\vec{q}\vec{r}} d\vec{q}$$

3. Rearrangement of the charge density:

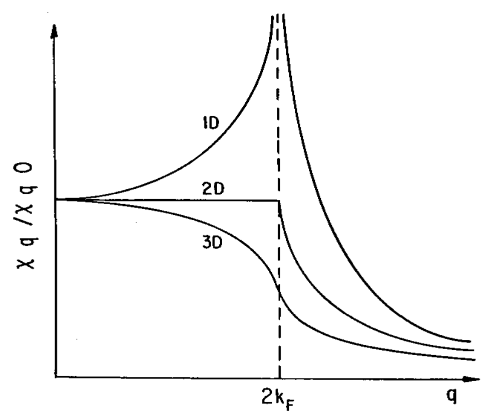
$$\rho^{ind}(\vec{q}) = \chi(\vec{q})\phi(\vec{q})$$

4. χ(q)–Lindhard response function:

$$\chi(\vec{q}) = \int \frac{d\vec{k}}{(2\pi)^d} \frac{f_k - f_{k+q}}{\varepsilon_k - \varepsilon_{k+q}}$$

In one dimension:

$$\chi(q) = \frac{-e^2}{\pi \hbar v_F} \ln\left|\frac{q + 2k_F}{q - 2k_F}\right|$$



$\chi(q)$ diverges at $q=2k_F$

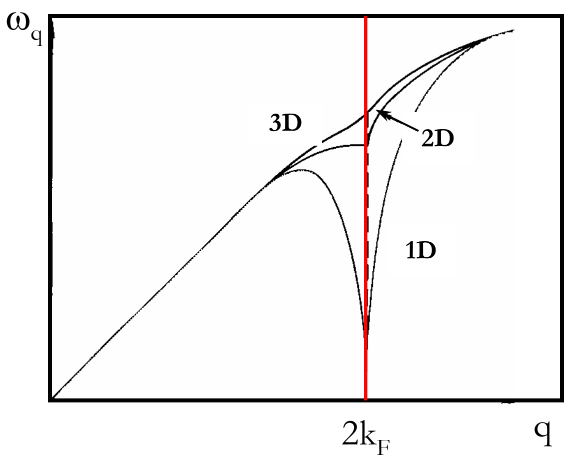
⇓

One-dimensional gas is unstable with respect to the formation of a periodically varying electron charge density

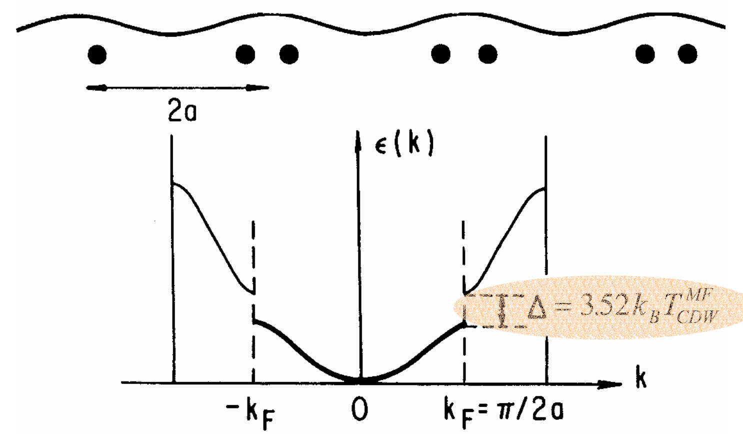
Consequences of charge modulation

/and electron-phonon coupling/

Modification of phonon spectrum
/Kohn anomaly or phonon softening at $2k_F$/

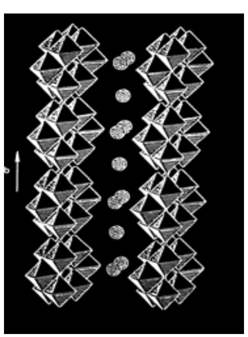


Periodic lattice modulation
and Pierls transition /opening of a gap at k_F/

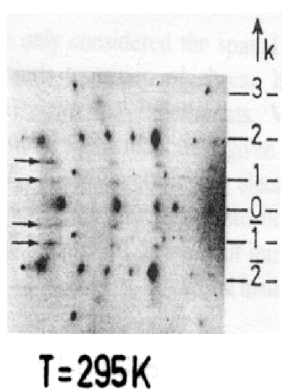


CDW in a real system: $K_{0.3}MoO_4$

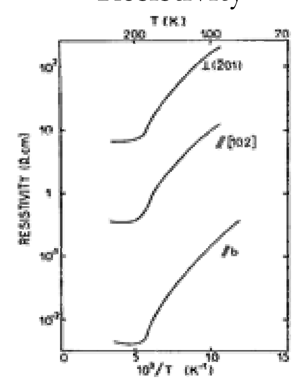
Quasi-one-dimensional crystal structure



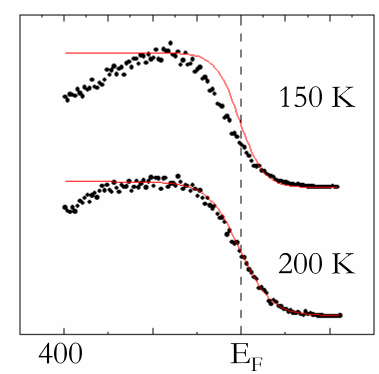
X-ray scattering



Resistivity



ARPES spectra at k_F



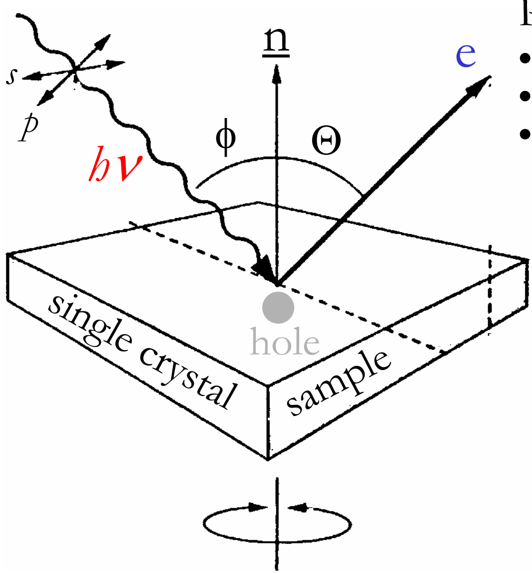
Angle Rsolved Photoemission
/band structure mapping/

Experiment

$$k_{//} = \sin\Theta \times \sqrt{2 \times m_e \times \eta^2 \times (h\nu - \Phi - E_{binding})}$$

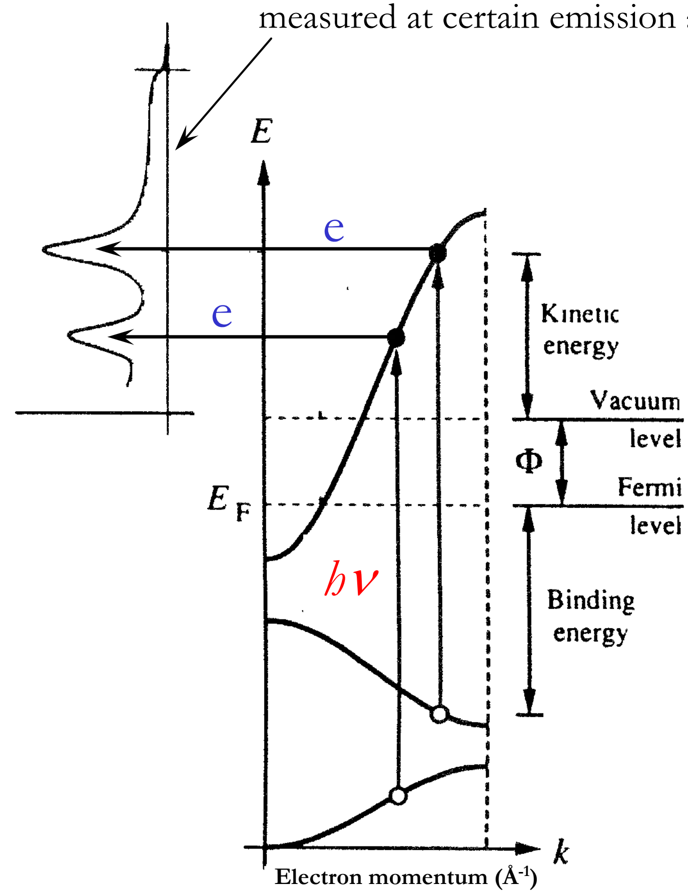
Data

Excitation Radiation
- photon energy
- polarization
- angle of incidence



Photoelectrons
- kinetic energy
- emission angle
- polarization

Energy Distribution Curves
(photocurrent vs. kinetic energy)
measured at certain emission angle

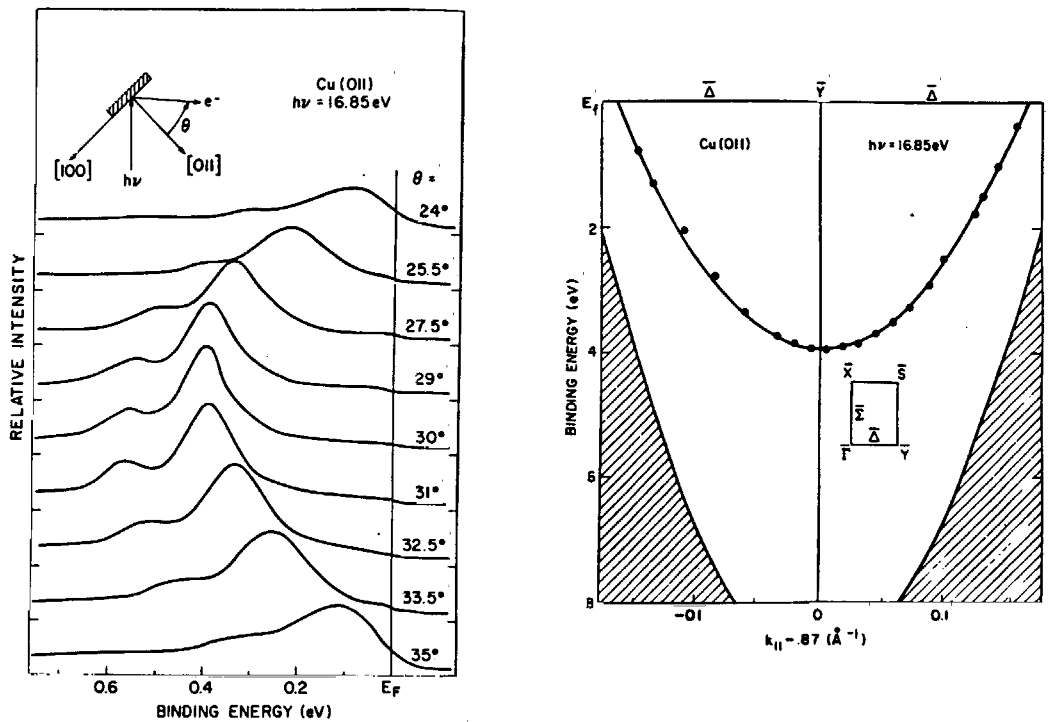


Important parameters:

Energy resolution (~20 meV)

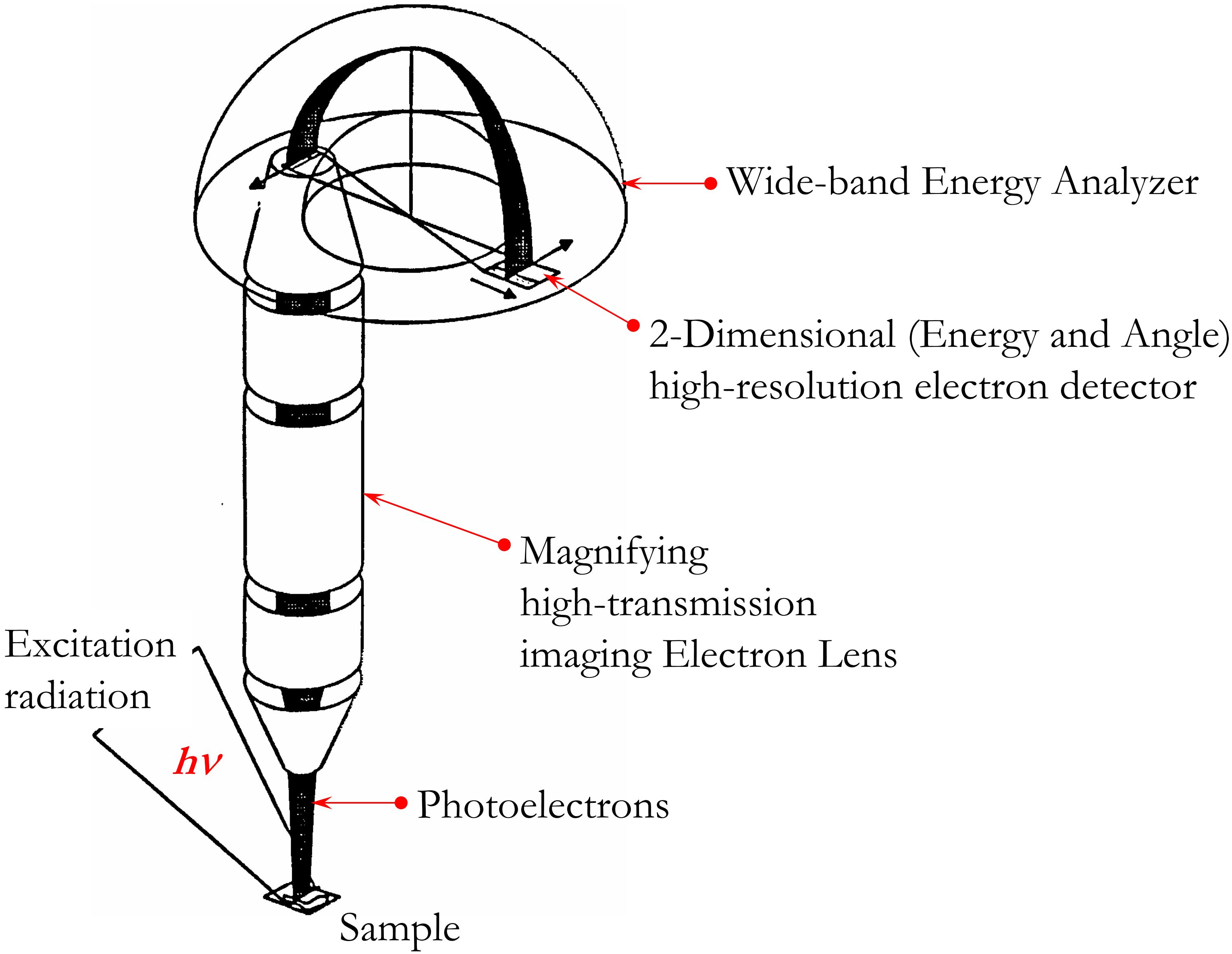
Angular resolution (~2°)

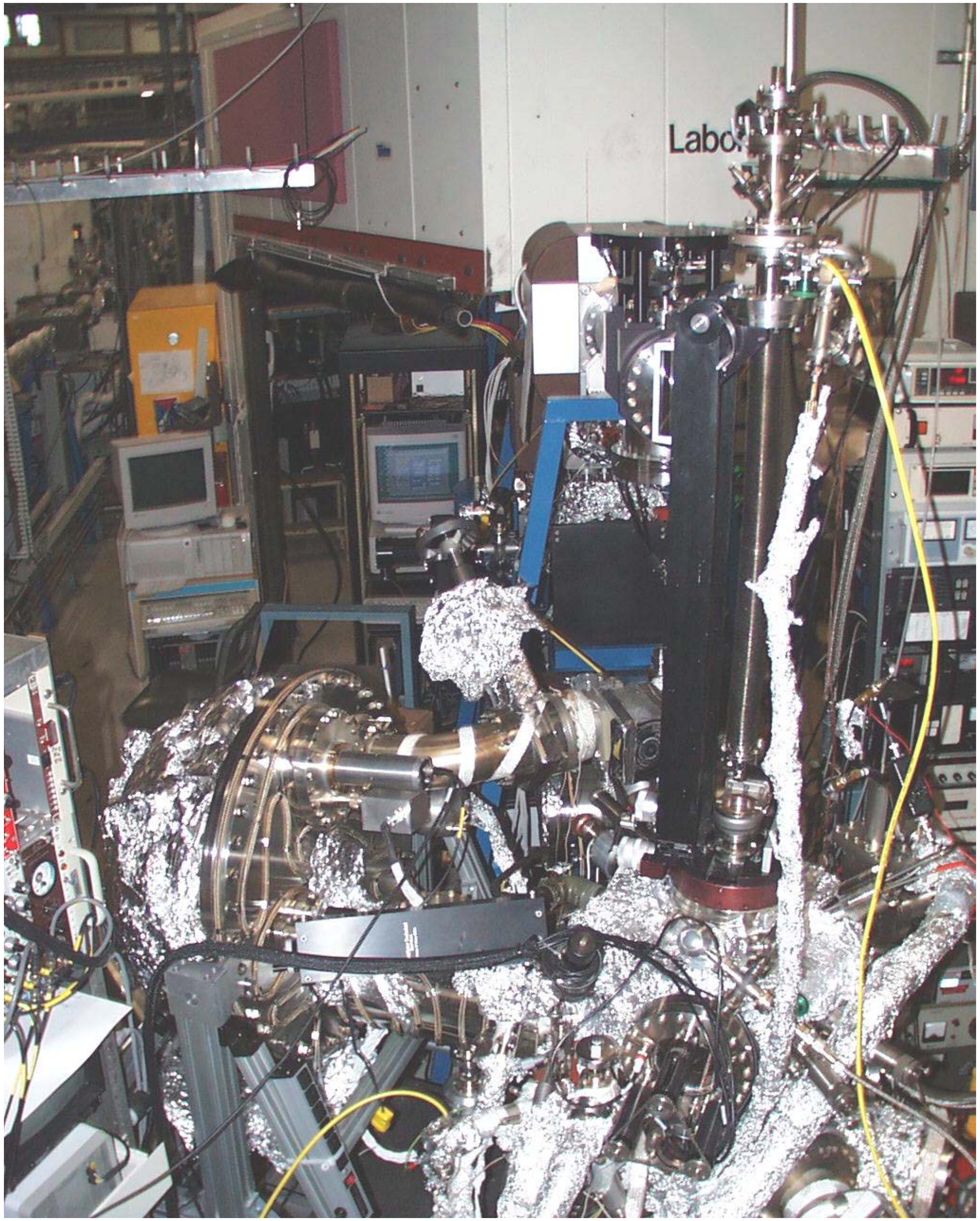
Surface State in Cu(011) mapped with ARPES
/S. Kevan, PRB **28**, 4822 (1983)/



New Instrumentation

/multi-channel detection in emission angle and kinetic energy/



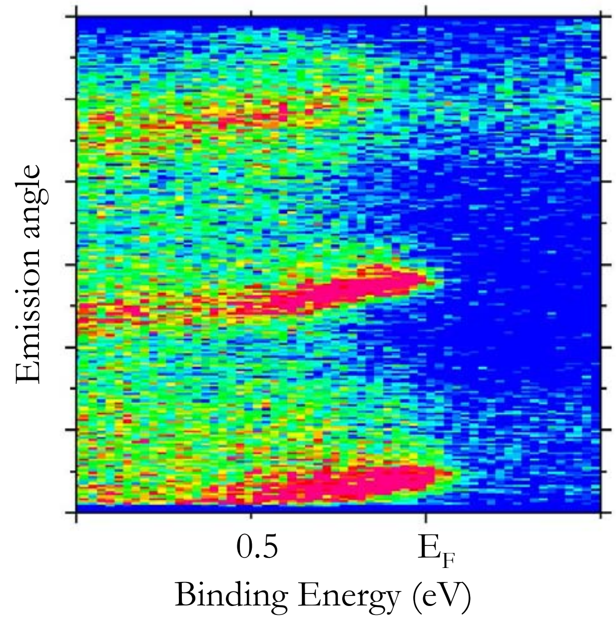


Experiment

ARPES chamber with Scienta 200-mm analyzer

Performance:

$\Delta E \sim 10$ meV
$\Delta\Theta \sim 0.2^{o}$
3×10^{-11} Torr



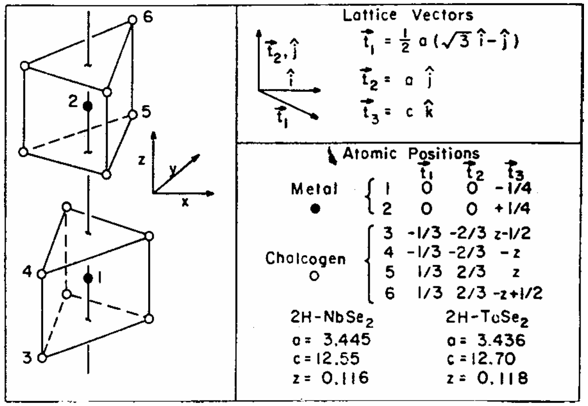
2H-$TaSe_2$: Motivations and Questions

✓ **CDW coexists with superconductivity:**
T_{CDW} ~ 122 K ; T_{SC} ~ 0.15 K

✓ **What drives the CDW transition:**
"Conventional" Fermi surface nesting or "saddle point" nesting?

✓ **CDW does not remove the entire Fermi surface:** What happens to the excitations at the Fermi energy in a presence of the CDW gap?

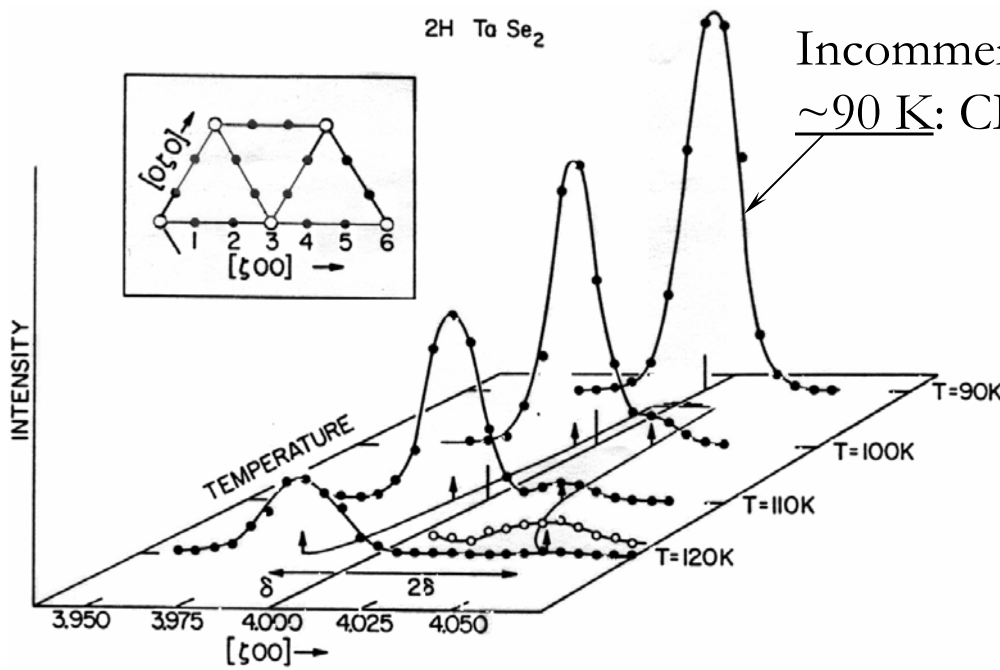
2H Crystal structure
/D.E. Moncton, J.D. Axe, and F.J. DiSalvo, PRB **16**, 801(1977)/



Neutron scattering experiment

/superlattice due to the Charge Density Wave/

D.E. Moncton, J.D. Axe, and F.J. DiSalvo, PRL 34, 734 (1975)



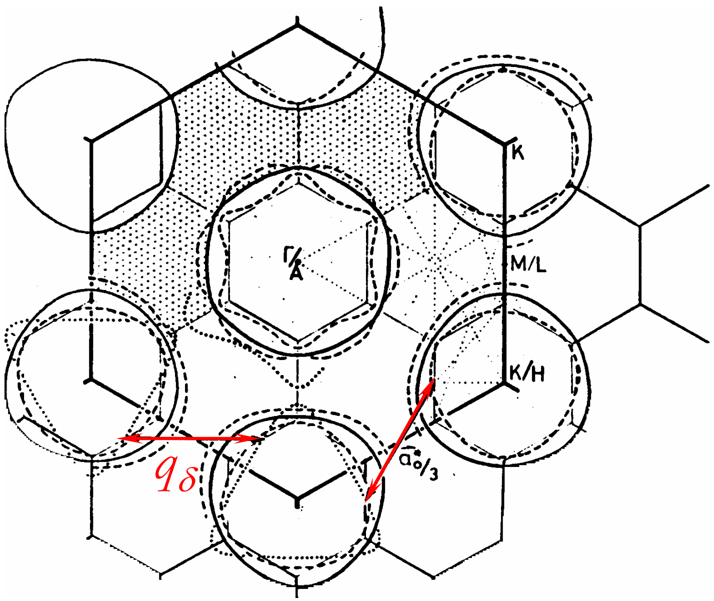
Incommensurate CDW: 122.3 K

~90 K: CDW locks to 3a superlattice

CDW wave vector: $q_\delta = 4\pi\,\{1-\delta(T)\}/a\sqrt{3}$

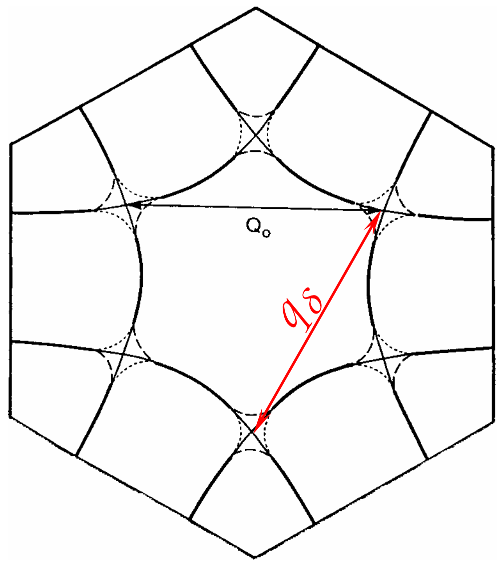
Nesting

A. Fermi surface nesting



J.A. Wilson, PRB 15, 5748 (1977)
G. Wexler and A.M. Wooley, J. Phys. C 9, 1185 (1976)
L.F. Mattheiss, PRB 8, 3719 (1973)

B. “Saddle point” nesting

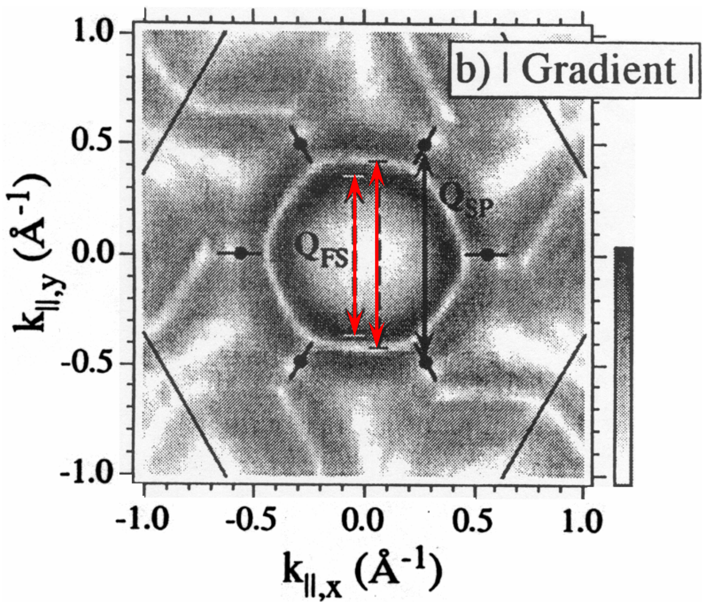


T.M. Rice and G.K. Scott, PRL 35, 120 (1975)

What is known?

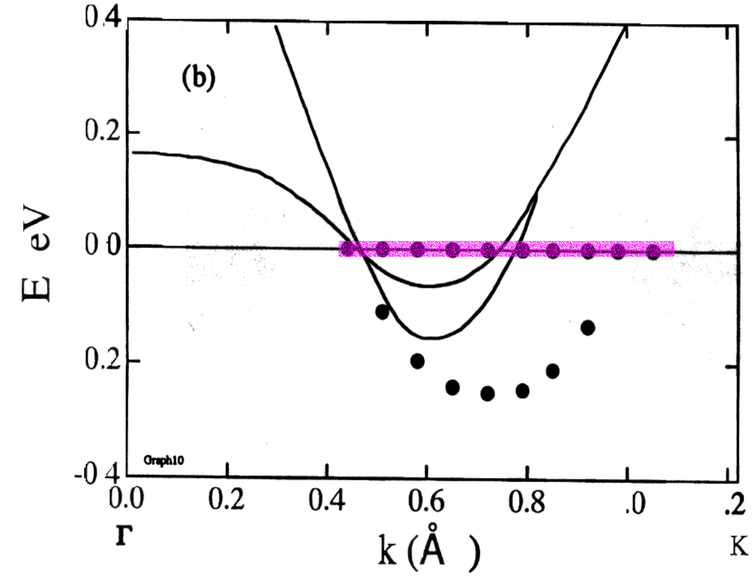
/ARPES studies/

A. "Regular" nesting



Th. Straub et al., PRL <u>82</u>, 4504 (1999)

B. Saddle band ⇒ Rice-Scott model

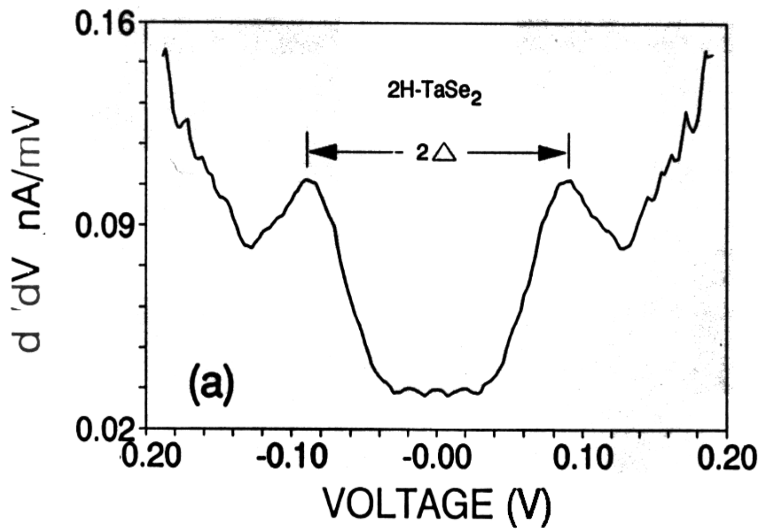


Rong Liu et al., PRL <u>80</u>, 5762 (1998)

$0.69\ Å^{-1} < q_\delta < 0.87\ Å^{-1}$ ⇐ **Problems** ⇒ Saddle band, not a point

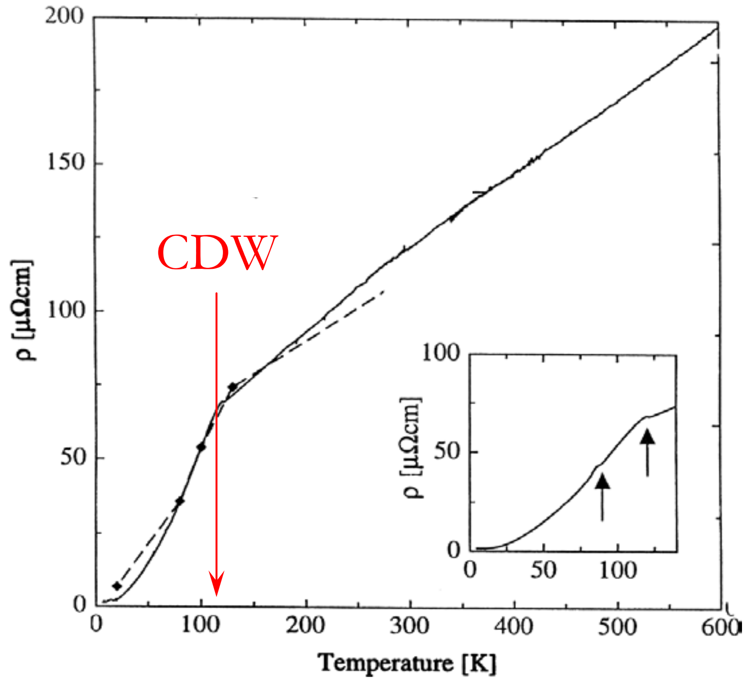
What does CDW do?

Opens up a gap, 2Δ ~ 150 meV
/STM data/



Z. Dai et al., PRB 48, 14543 (1993)

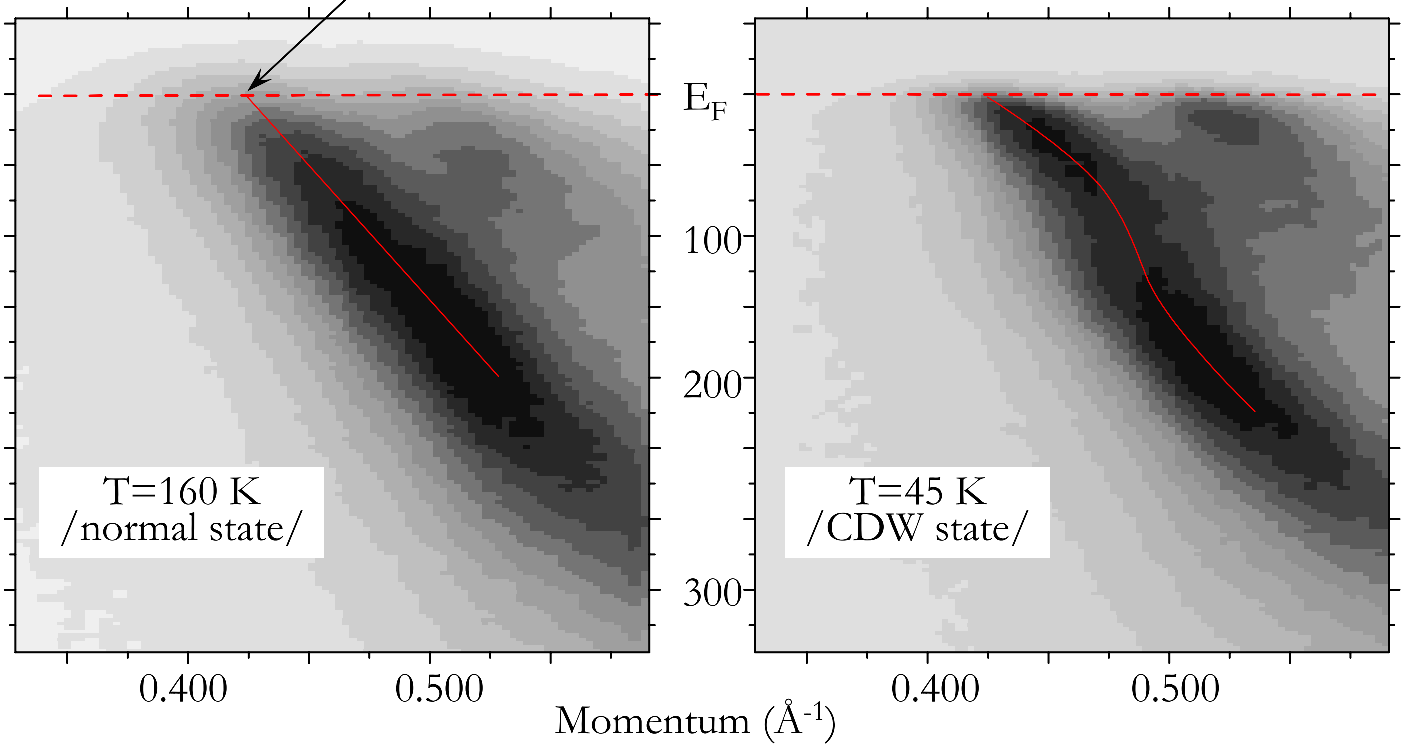
Freezes out scattering channels
/transport measurements/

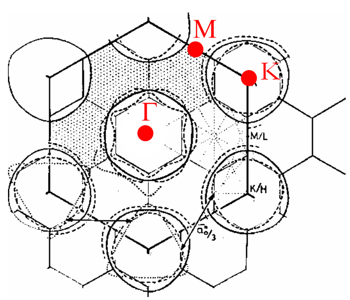


V. Vescoli et al., PRL 81, 453 (1998)

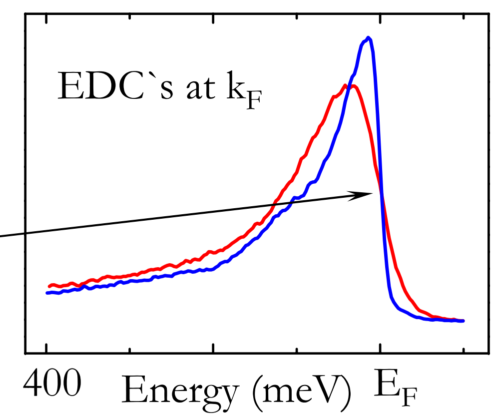
Band mapping along ΓM

Fermi level crossing: $k_F = 0.425$ Å^{-1}

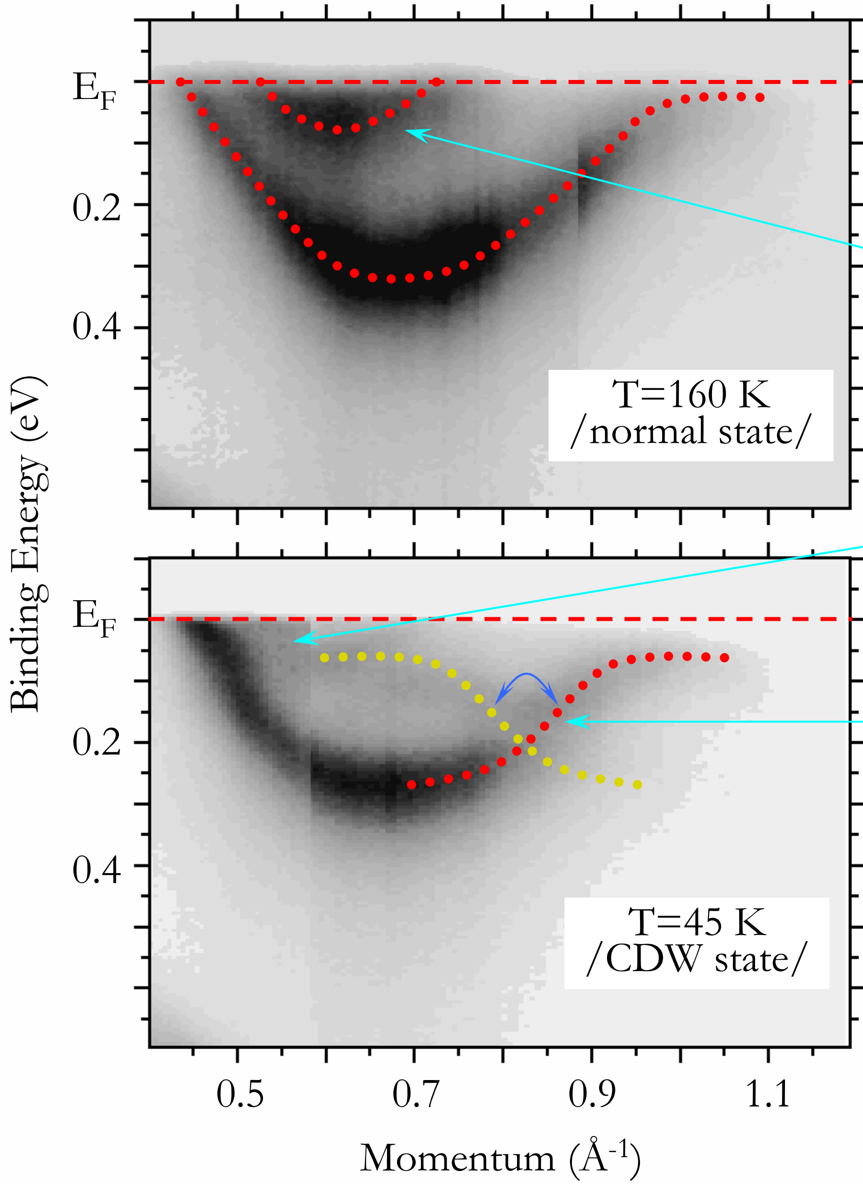




Nesting along ΓM
is not very good
and there is no gap
at the Fermi level...



Band mapping along ΓK



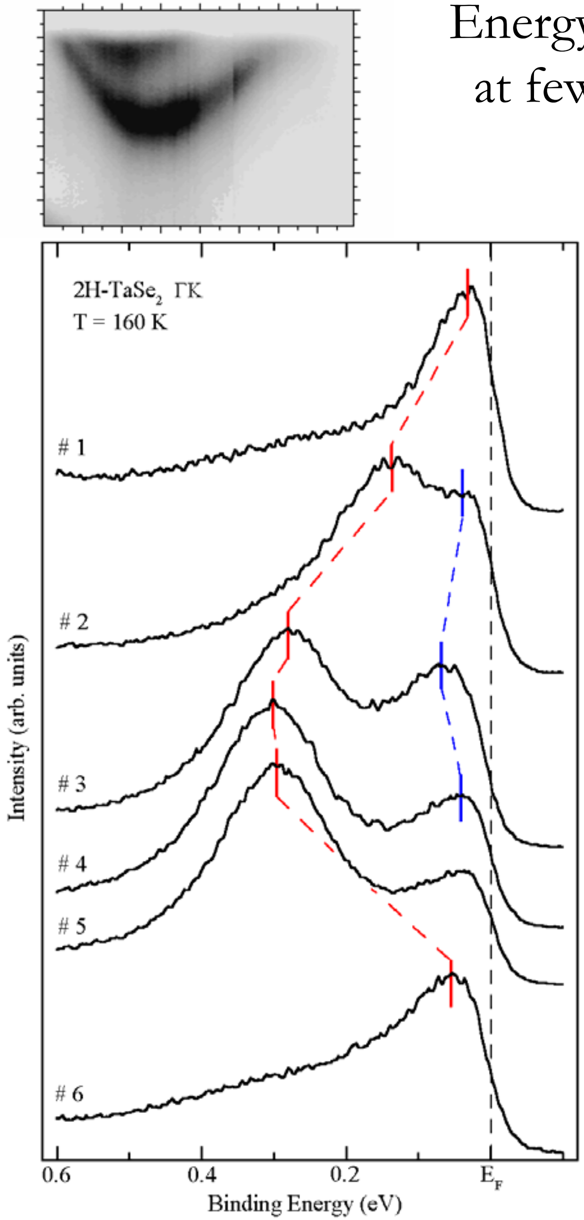
New results:

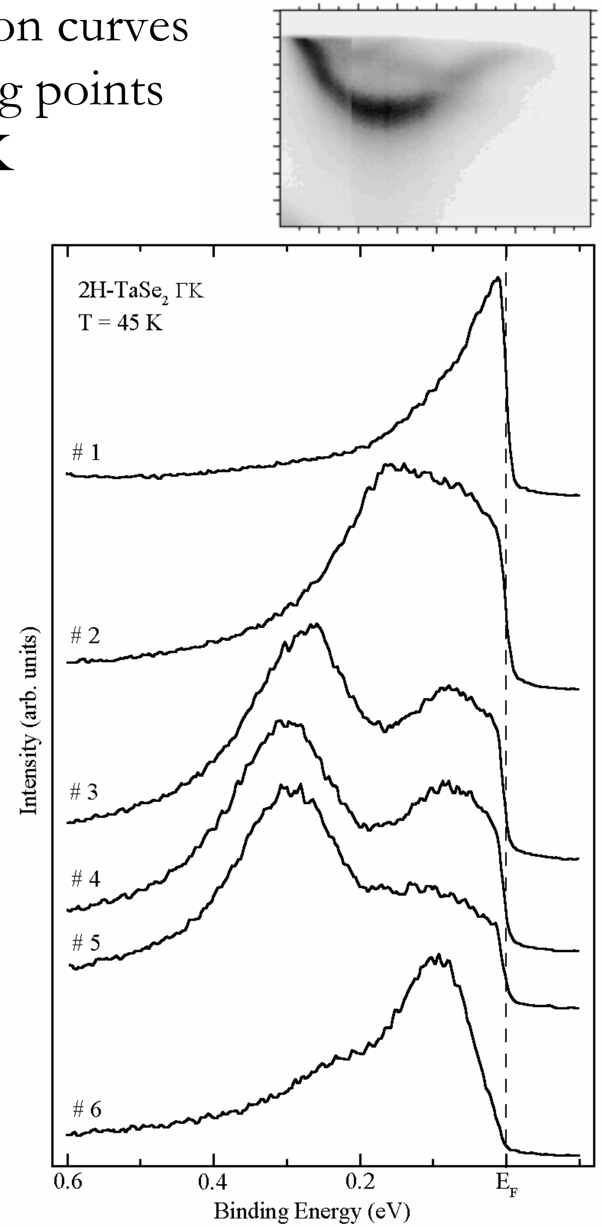
- Saddle point has a bandwidth of just ~50 meV and extends for only 0.2 Å^{-1}
- It is no longer there in the CDW-state
- Band "folds back" at ~0.825 Å^{-1}; This projects into ~2/3 of ΓM

★

These observations point towards the Rice-Scott model

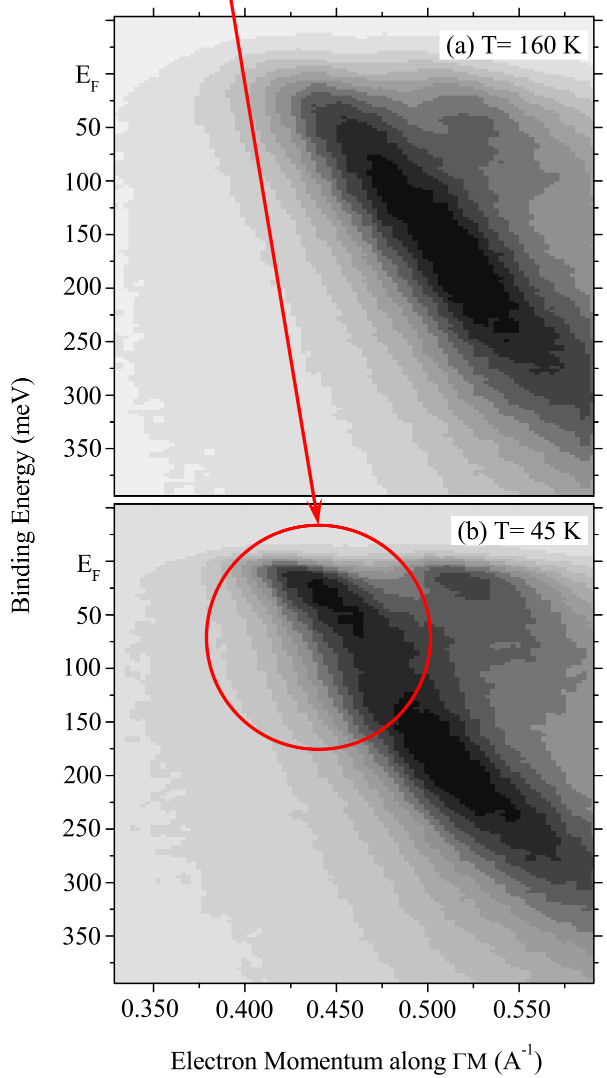
Energy distribution curves at few interesting points along ΓK

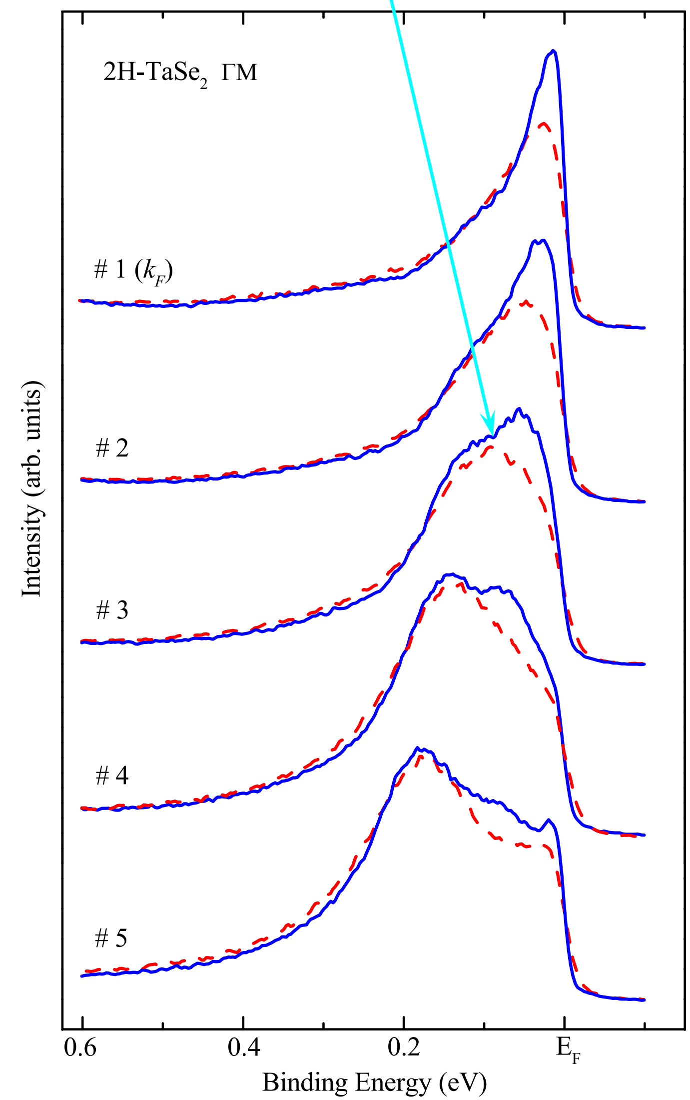




How does CDW affect low-energy excitations?

At **45 K** coupling of quasiparticles to the collective mode of some sort manifests itself via changes of both, ARPES **line-shapes** and **dispersion relations**

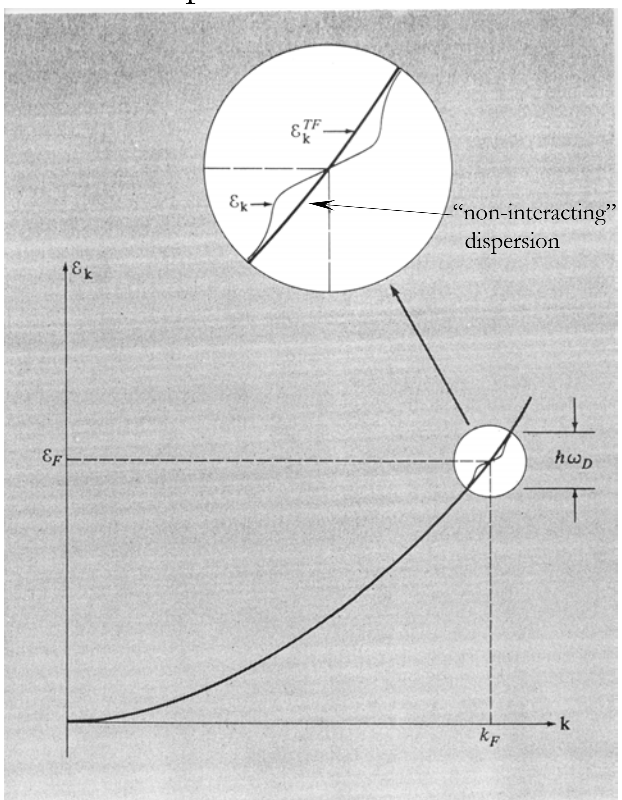




Electron-phonon coupling

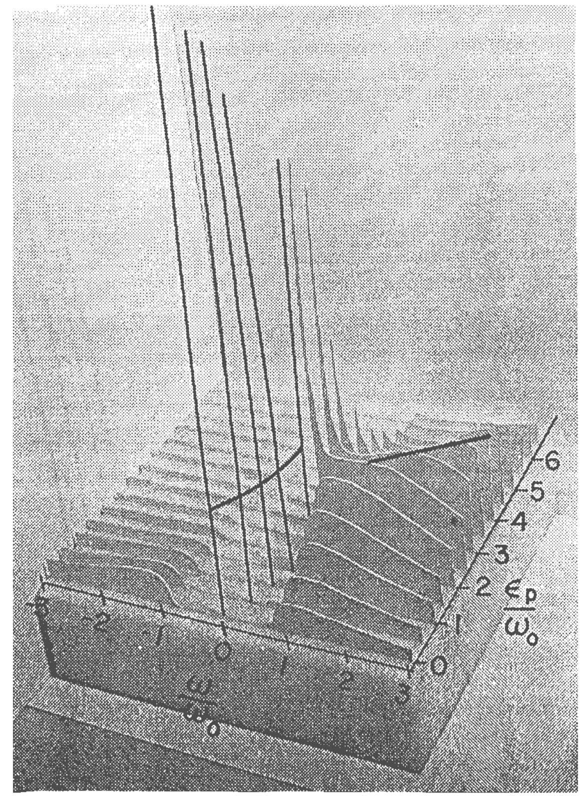
$$\textit{Spectral function: } A(k,\omega) \sim \frac{|\operatorname{Im}\Sigma(k,\omega)|}{\left[h\omega - e_k - \operatorname{Re}\Sigma(k,\omega)\right]^2 + \operatorname{Im}\Sigma(k,\omega)^2}$$

Dispersion relations



Solid State Physics
Neil W. Ashcroft
N. David Mermin

Spectral functions



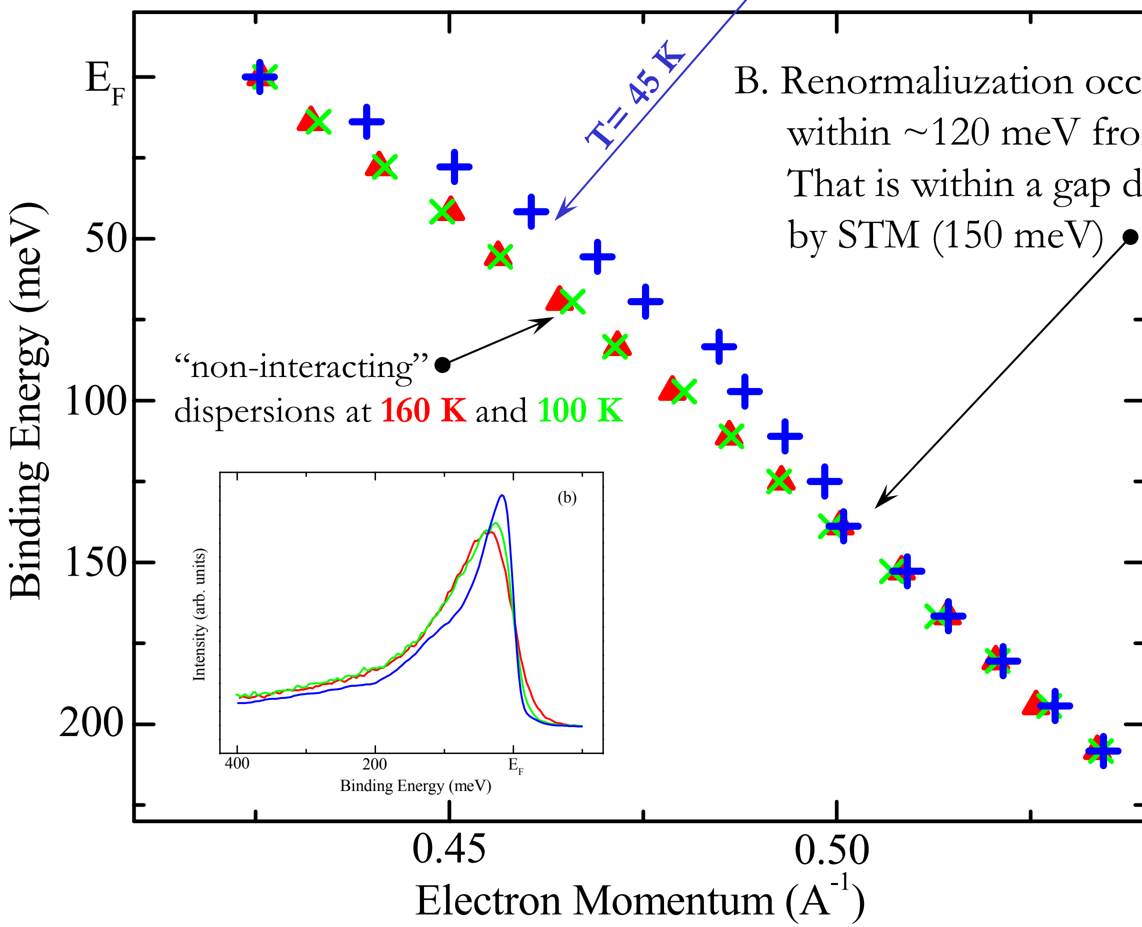
Douglas J. Scalapino
in Superconductivity,
R.D. Parks, editor

What is this collective mode?

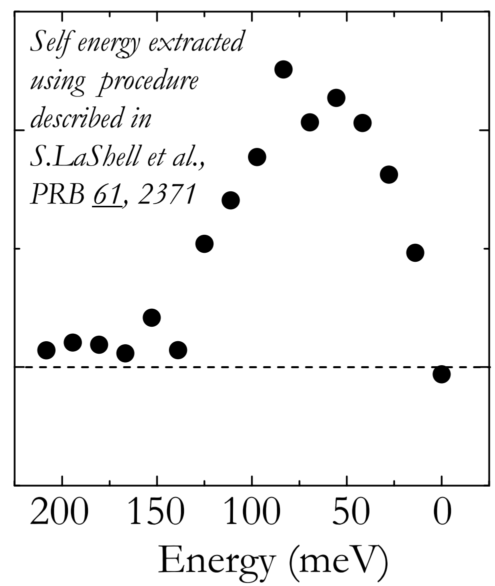
/a few clues from dispersion relations/

A. When CDW is commensurate with the lattice
"Renormalization" of dispersion becomes obvious

B. Renormaliuzation occurs
within ~120 meV from E_F
That is within a gap detected
by STM (150 meV)



C. Real part of the self energy
peaks at ~80 meV, again
within a CDW gap



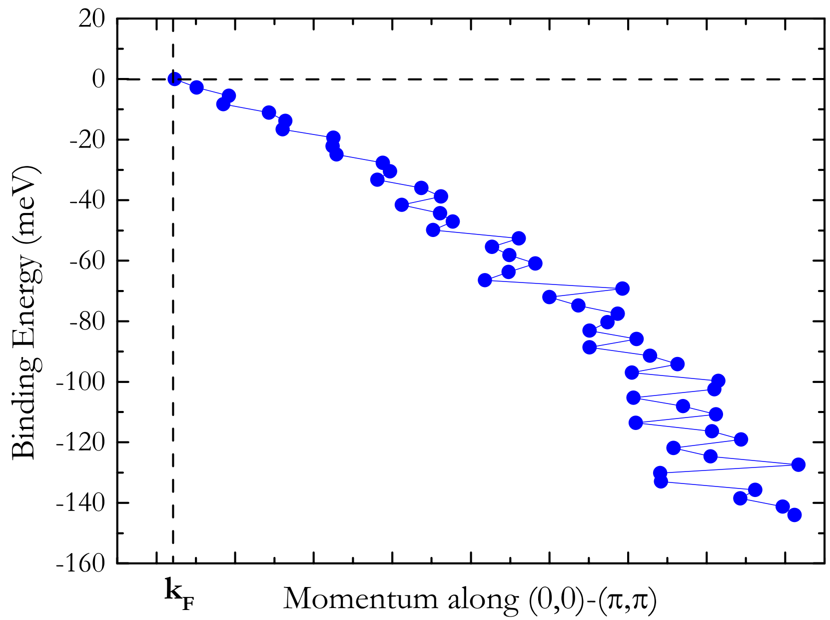
It may be an exciton-like mode

Is 2H-$TaSe_2$ similar to the HTSC?

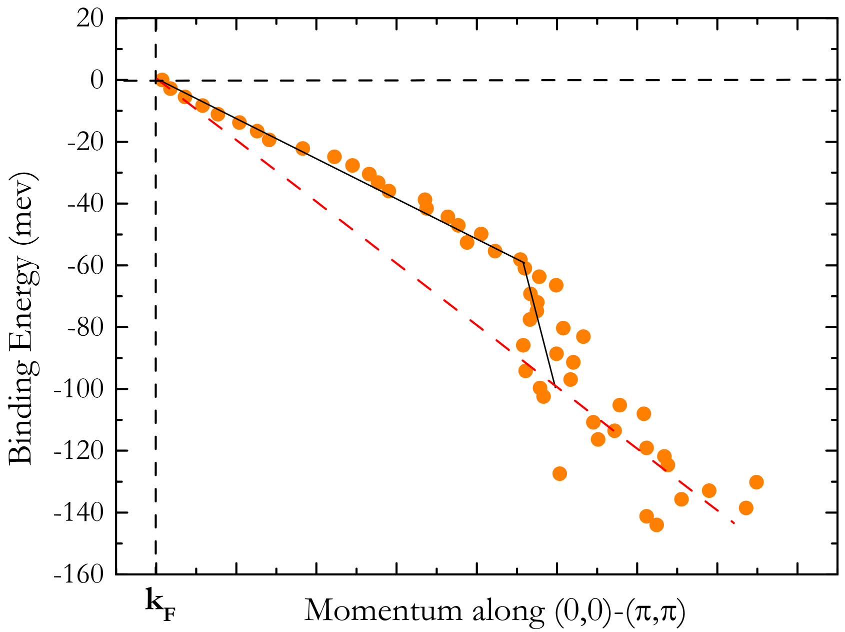
/of course not, however…/

Dispersions relations in underdoped (T_C=80 K) $Bi_2Sr_2CaCu_2O_8$
along (0,0) to (π,π) /gap node/

A. Normal State, T=120 K

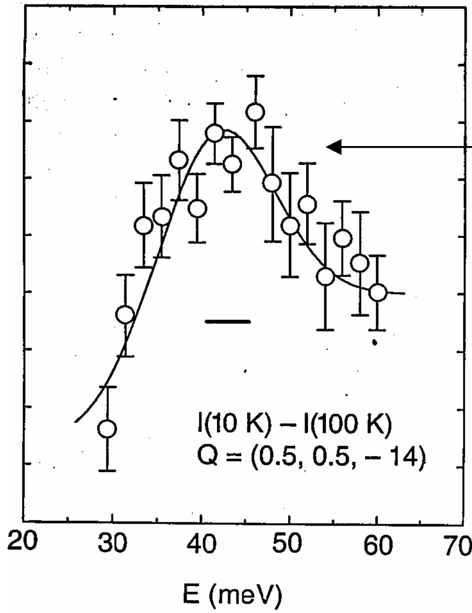


B. Superconducting state, T=45 K



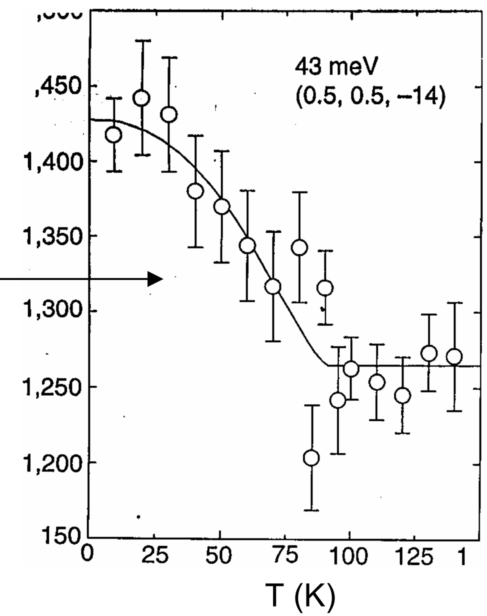
Neutron scattering from Magnetic excitations in $Bi_2Sr_2CaCu_2O_8$

/H.F. Fomg et al., Nature 398, 588 (1999)/



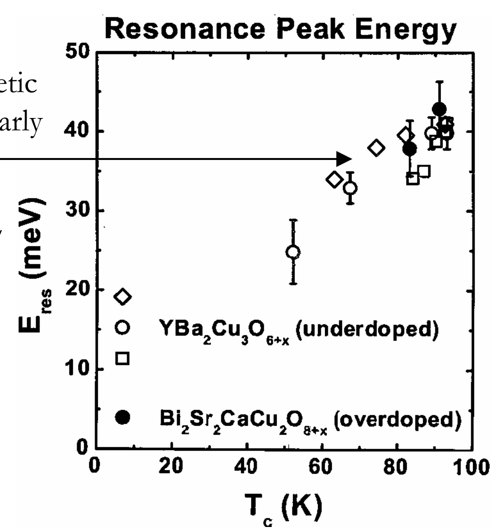
Energy profile

Temperature dependence



Energy of the magnetic excitation scales linearly with Tc

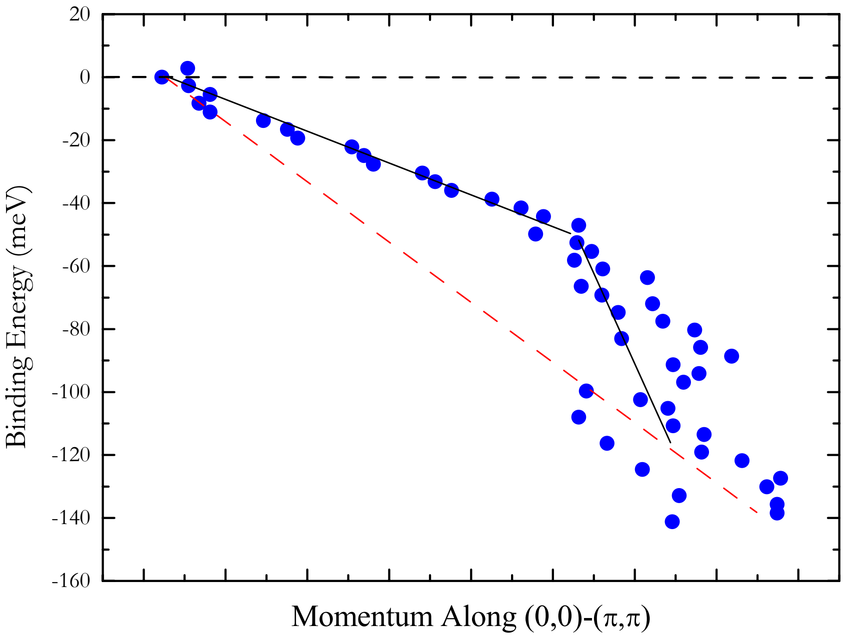
/H. He et al., cond-mat/0002013/



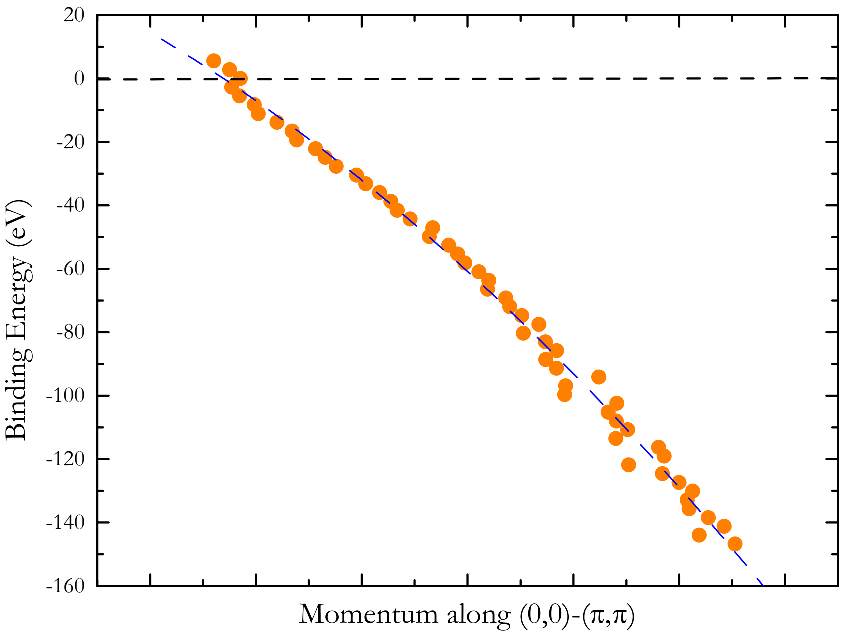
What will we see in ARPES?

Preliminary results on underdoped (Tc=69 K) and overdoped (Tc=51 K) $Bi_2Sr_2CaCu_2O_8$ samples

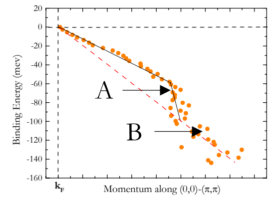
A. Superconducting State, T_c=69 K

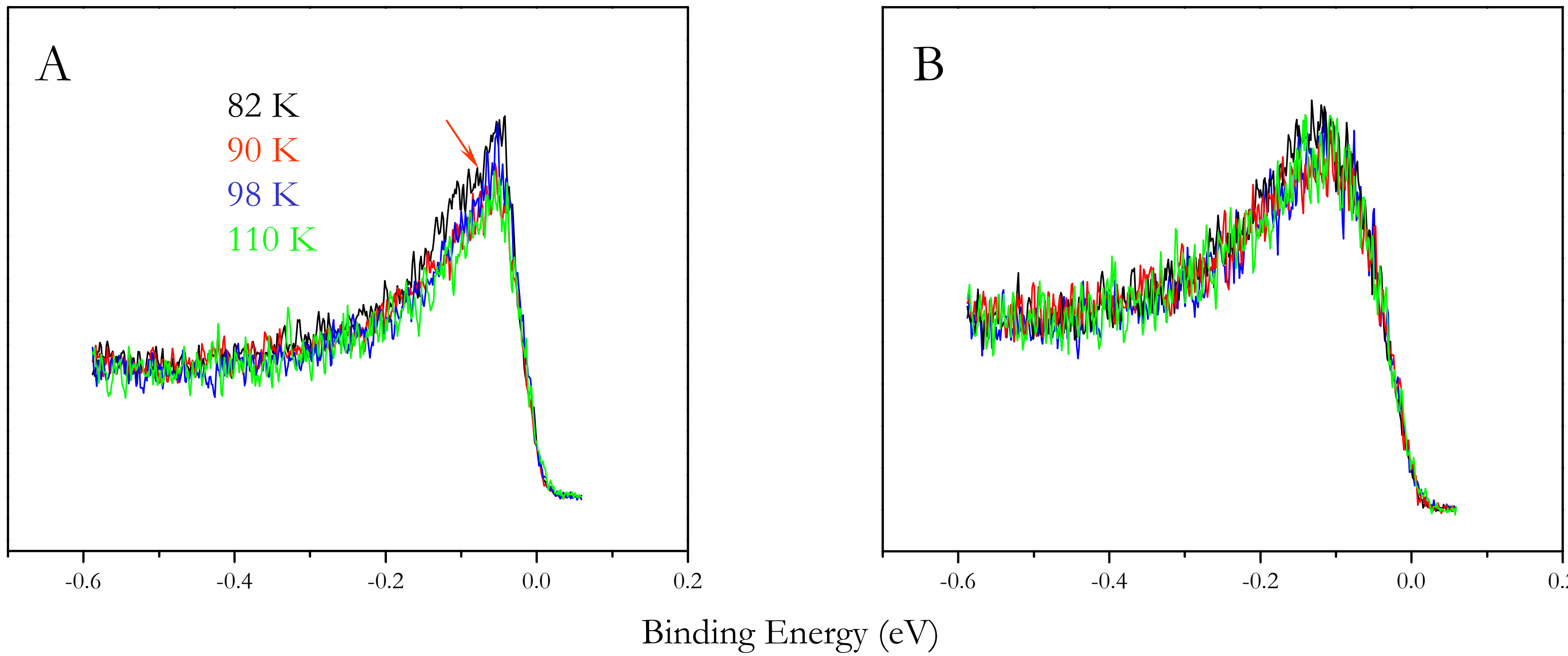


B. Superconducting state, T_c~51 K



Optimally doped BISCO (T_C=91K)
/spectra at different temperatures/



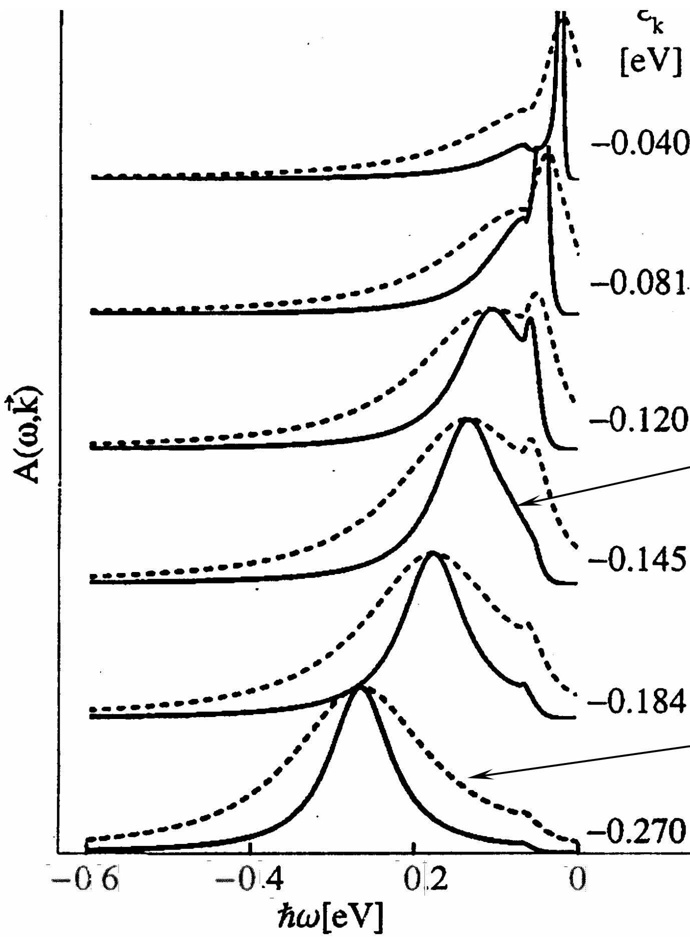


Spectra taken above T_c or at high binding energies do not exhibit temperature broadening
P. W. Anderson: spin-charge separation as a source of "quantum protection" in HTSC /Science 288, 480 (2000)/

What about impurity scattering?

Broadening due to the impurity scattering

/LaShell et. al., PRB 61, 2371 (2000)/



ARPES study of surface state in Be(0001): strong electron-phonon coupling case

Spectral functions in the Debye model (ω_D=65 meV, λ=0.65)

Impurity broadening

Future measurements

CDW in transition metal dichalcogenides as a model of stripe ordering in high critical temperature superconductors?

2H-$NbSe_2$
/superconductor at ~7K, no lock-in CDW state/

2H-$TaSe_2$ with defects
/suppression of lock-in CDW transition, T_c rises up to ~4K/